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The Kinetics of Insecticide Action. Part V: Deterministic Models to Simulate the Movement of Pesticide from Discrete Deposits and to Predict Optimum Deposit Characteristics on Leaf Surfaces for Control of Sedentary Crop Pests*

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Abstract: Mathematical models have been used to identify combinations of deposit size, density and concentration which result in effective control of sedentary crop pests using minimal amounts of insecticide. A model based on point source diffusion gave an adequate description of the spread of biocidal areas around deposits with time; the more complex disc source model gave similar results. The point source model has been developed further to investigate how pesticide inputs might be reduced while maintaining adequate control. Models based on the cumulative effects of toxicant with time gave marginally better fits in the tails of the tolerance distribution. Prediction of LN_{50} values using a model which takes account of overlapping biocidal areas was in reasonable agreement with experimental results. Models which have been developed to investigate the factors which affect the control of sedentary crop pests by insecticides and acaricides may also be used to predict optimal spray patterns for contact herbicides and fungicides.

Key words: deterministic models, optimal deposits, sedentary pests, pesticides, biocidal areas

1 INTRODUCTION

Current concerns about pesticide usage suggest that inputs of chemical control agents need to be significantly reduced. This is particularly true for situations where integrated pest management (IPM) is applicable. IPM requires minimal agrochemical use in order to provide opportunities for populations of insect predators to exercise biological control. Mathematical modellings offers the prospect of precise definition of those spray deposit characteristics which lead to effective control of the pest, but present little hazard to the biological control agent.

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Earlier papers in this series have highlighted the role of pharmacokinetics and pharmacodynamics in determining the inherent toxicity of insecticides[1–3] and have investigated how computer simulations can take account of these processes to predict the levels of control of mobile insect pests which can be achieved for particular deposit characteristics.[3] This paper addresses the problem of controlling sedentary arthropod pests.

1.1 The concept of biocidal area

Studies to investigate the control of whitefly larvae *Trialeurodes vaporariorum* (Westwood) have established that each deposit of permethrin is surrounded by a region where there is a high probability of mortality, even though these sedentary organisms have not been

contacted by direct impact of insecticide.[4–7] For modelling purposes, this region of control may be regarded as a circular zone around the deposit within which there is a probability of kill $P > 0{\cdot}5$; each zone is termed a biocidal area;[8] the radius of the biocidal area may be termed r_{50}.[9]

Munthali[8] and Munthali and Scopes[10] developed the idea of biocidal areas in studies which they performed to assess the effectiveness of different-sized deposits of the insecticide dicofol produced by controlled droplet application (CDA) for the control of the eggs of *Tetranychus urticae* (Koch) on tobacco leaves (*Nicotiana tabacum* L. cv. Brazilian Blend). Munthali compared the change in LD_{50} (measured as the amount of active ingredient (AI) per cm^2 necessary to elicit 50% control) as drop size and concentration varied.[8] The LD_{50} values (ng cm^{-2}) can be inverted to give biocidal efficacies (cm^2 ng^{-1}) which describe the area of median control which is achieved per unit mass of AI.[11] Biocidal efficacy is therefore related to biocidal area.[9] Biologically efficient, cost-effective treatments have deposit patterns with large biocidal efficacies. Munthali showed an optimum concentration (approximately 10 g $litre^{-1}$) for dicofol against red spider mite eggs on tobacco leaves which resulted in a maximum biocidal efficacy. The observed optimum concentration decreased with increasing deposit size.

The establishment of biocidal areas has been modelled using analytical equations based on point and disc source diffusion.[9,12] Such models assume that pesticide moves out from each deposit to establish a biocidal area within which local control of the pest is achieved. Sharkey *et al.*[9] suggest that the overall control achieved on a treated surface depends on the summed effect of all the biocidal areas on that surface. The models predict how time, concentration of AI, deposit number per unit area and deposit size (the determining variables) influence the size of the biocidal area and hence the area of leaf protected per unit mass of pesticide (the biocidal efficacy). Because the transfer functions describing the movement of pesticide and the distribution of the tolerances of the pest to the pesticide are non-linear, the changes in effectiveness which result from adjustments to the determining variables cannot be predicted intuitively or empirically. The models can be used, however, to identify which combinations are optimal for a given control situation.

1.2 Cumulative biocidal areas

Sharkey *et al.*[9] considered how concentration, droplet size and drop density related to the area of leaf cover protected to a given level of control. Assuming negligible overlap of the regions of influence around the insecticide deposits, they showed that the cumulative biocidal area (CBA; the total leaf area protected to at least 50% control per unit mass of AI) can be written:

$$\mathrm{CBA} = \frac{\pi r_{50}^2}{m} N R_f \tag{1}$$

where,

r_{50} = the radius of the biocidal area around a deposit i.e. the region within which there is at least 50% response,

m = mass of active ingredient in the deposit at time $t = 0$,

N = number of monosized droplets of radius a that can be formed from a given volume of spray L,

and

R_f = retained fraction of spray on leaf surface

According to Sharkey *et al.*[9] the CBA may also be expressed as:

$$\mathrm{CBA} = \frac{9LDtR_f}{4\pi a^6 C_0}\left[\ln\left(\frac{C_0 a^3}{3Dt10^6}\right) - \mu\right]10^{21} \tag{2}$$

This result has been derived assuming that a point source pesticide transfer model can adequately describe the increase in biocidal areas with time. For given values of the diffusion coefficient D, inflight droplet radius a, mean of the log tolerance distribution μ and time t after placement of the deposits, the variation of CBA as a function of C_0 can be investigated. For example, using standard mathematical methods it can be shown[9] that the optimum concentration C_0' is independent of time; that C_0' decreases with increasing drop size; that there is a maximum CBA which is independent of time t and that the maximum CBA increases with decreasing droplet radius a. These features are consistent with the results obtained by Munthali for control of eggs of *T. urticae* using dicofol.[8,10] The properties of the CBA model (eqn (2)) are therefore similar to those observed for biocidal efficacy,[8,10] although, as the present paper shows, the formulation of the latter is different.

This paper reports further development, evaluation and validation of the models and describes examples to show how mathematical modelling may be used to identify optimal deposit requirements for effective treatment. The results suggest that more effective treatments for the control of pests and diseases with required persistence of effect and minimal impact on beneficial organisms are possible using reduced amounts of AI.

2 MATERIALS AND METHODS

2.1 Mathematical

The mathematical forms of both the point source and disc source models have been quoted without proof

from Crank[12] and the modifications made to these models are undertaken using standard mathematical methods.

2.2 Computational

In-house software was written and implemented on a 286 ICL PC to enable good initial estimates of parameters prior to model fitting using the BMDP[13] Derivative Free Non-linear Regression Program AR mounted on a VAX.

2.3 Biological data

The biological data, describing the control of red spider mite and whitefly larvae by residual treatments applied by ULV, have been reported by Munthali,[8] Munthali and Scopes,[10] Abdalla[4] and Adams *et al.*[7]

2.4 Chemicals

Solutions of technical permethrin (*cis* : *trans* ratio = 60 : 40 w/w) from 10 to 200 g litre^{-1} were prepared in an oil-based carrier VK1 (Timmer Ltd) which contains a low-volatile polar solvent plus a low-volatile paraffin. An additional oil-based formulation JF8133, containing a volatile polar solvent plus a low-volatile and a very low-volatile paraffinic solvent, was supplied as 100 g litre^{-1} permethrin (Zeneca, Jealott's Hill). Each spray solution contained 'Uvitex' OB fluorescent tracer (5 g litre^{-1}) and was stored in a sealed glass tube at 1°C.[7]

3 RESULTS AND DISCUSSION

3.1 Predicting chemical control using point and disc source diffusion models

The bioassay results for two experimental formulations of permethrin (JF8133 and VK1) applied at a variety of drop sizes and concentrations are presented in Fig. 1 as plots of the proportion mortality observed at four days versus radial distance from the deposit centre. These are characterised by high mortality (100%) near the deposit perimeter, which declines as the distance from the deposit is increased to reach levels consistent with control mortality at longer radial distances. The zones of control described in Fig. 1 occupy larger areas than the spread droplets which have impacted on the leaf surface, suggesting that pesticide has moved out from the perimeter of the deposit down a gradient of concentration as a result of random molecular motion (e.g. by diffusion or imbibition). The zone of control with a radius (r_{50}) such that the probability of mortality within the outer zone perimeter is equal to or greater than 50% is termed the biocidal area ($P > 0{\cdot}50$).[9]

A mathematical model describing the establishment of biocidal areas has been derived assuming random movement of insecticide away from a point source representing the deposit.[9] Equation (1) of Sharkey *et al.*[9] can be used to predict the masses per unit area at different radial distances from the deposit and hence the probability of death (eqn (17))[9] at these distances. In the earlier study, regressions were undertaken using the standardised *z*-scores of the observed proportion response as the dependent variable. Several modifications to the procedure of Sharkey *et al.*[9] have now been introduced and the predictive power of the revised mathematical formulation investigated.

The observed proportion response can now be fitted directly so that transformation to *z*-scores (eqn (17))[9] is

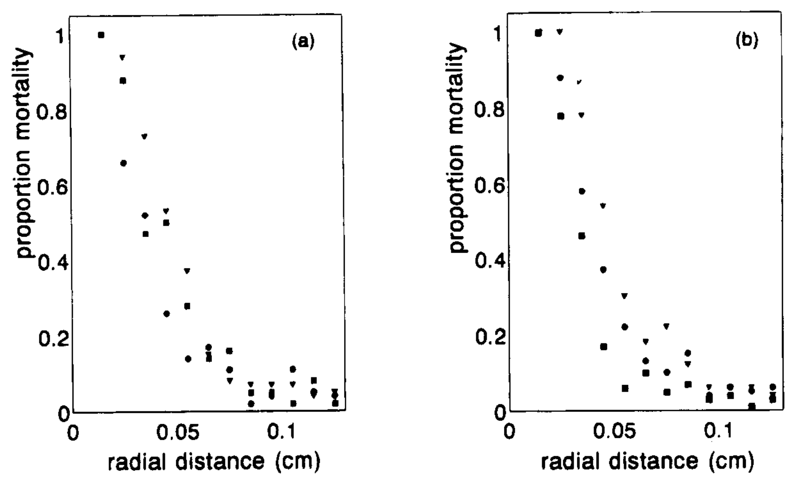

Fig. 1. Mortality response of whitefly larvae to CDA applications of permethrin in different commercial formulations as a functions of distance from the deposit centre to indicate the zones of control: (a) JF8133 formulation: 100 g litre^{-1} concentration for (●) 59, (▼) 108 and (■) 114 μm deposit diameter; (b) VK1 formulation: (■) 50, (●) 100 and (▼) 200 g litre^{-1} concentrations for 107, 110 and 113 μm deposit diameters, respectively.

unnecessary. Furthermore, the predicted mortality, P_{pred} at a radial distance r and time t, is corrected for the natural responsiveness of the whitefly larvae using the appropriate form of Abbott's correction:

$$P_{pred} = P_{ins}(1 - P_{control}) + P_{control} \tag{3}$$

where,

$$P_{ins} = Q\left\{\frac{\log[C^*(r, t)] - \mu}{\sigma}\right\} \tag{4}$$

and $Q(\cdot)$ is the standard normal cumulative distribution function, $C^*(r, t)$ is the mass per unit area evaluated at radial distance r and t (eqn (1) of Sharkey *et al.*[9]), P_{ins} is the predicted mortality at a radial distance r and time t resulting from the insecticide, and $P_{control}$ is the predicted control mortality at large radial distance from the deposit centre. Equation (3) therefore replaces eqn (17) of Sharkey *et al.*[9]

The probability of death, P_{pred}, estimated from the masses per unit area at different radial distances from the deposit (eqn (1) of Sharkey *et al.*[9]), can be obtained by fitting eqn (3) to the observed proportion mortality for given values of the diffusion coefficient, which is a parameter in the model, and time, which is treated as a fixed variable, using a non-linear regression procedure. The radial distances at which the observations were made are substituted into the point source diffusion model (eqn (1))[9] to calculate the concentrations of pesticide at these radial distances. The logged values of the pesticide concentrations, together with values of the mean and standard deviation of the tolerance distribution, are then used to generate the area under a normal curve using the computer routine of Cook, Craven and Clarke;[14] this area represents the proportion of organisms responding. The regression procedure provides estimates of the diffusion coefficient and the mean and standard deviation of the tolerance distribution.

It was initially felt that the fits to the data might be improved by using the more complex disc source model, given by eqn (18) of Sharkey *et al.*,[9] in the regression. However, as can be seen in Fig. 2, where the results for both the point source and disc source models are superimposed on a plot of the obseved mortality profile, there is little difference between the predictions of either model. The similarity between the models was reproduced for all drop sizes and concentrations, even though the form of the disc source model is very different to that of the point source model. The fact that both models produce more or less identical response profiles is made possible by different optimal values for the parameters (and in the case of the mean and standard deviation of the tolerance distribution, different units) of the models (Table 1). Work is now under way to confirm the estimated transport coefficients by experiment.

3.2 Modelling the cumulative effects of applied chemical over time

An implicit assumption of both the point and disc source models is that the mortality at a fixed time and radial distance from the centre of a deposit results from the concentration of AI measured at that time and distance. Clearly, the effect of the diffused insecticide at a defined point is not simply the effect of its concentration at a particular time, but rather, there is an accumulated effects of changes in concentration at that point from the time the deposit arrives on the surface to the time at which mortality is recorded. This idea is more easily realised by viewing a plot of the concentration of diffused material from the deposit as a function of time after placement and radial distance from its centre (Fig. 3). Although the concentration of pesticide inside the deposit perimeter continues to reduce over time, for points just outside the perimeter, concentration rises and falls with time. At longer distances from the deposit

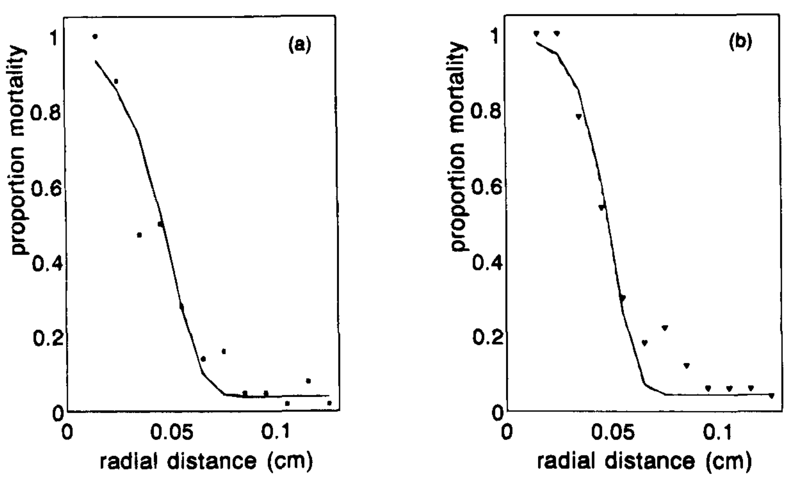

Fig. 2. Disc and point source models (see text for details): (a) JF8133 formulation: 100 g litre^{-1} concentration for 114 μm deposit diameter; (b) VK1 formulation: 200 g litre^{-1} concentration for 110 μm deposit diameter.

TABLE 1
Estimates of Transport Coefficients, LD_{50} Values and Standard Deviations of Tolerance Distributions of Whitefly for Two Formulations of Permethrin Derived Using Different Models

	Point (*log* (*ng cm*$^{-2}$))	*Disc* (*log* (% *w/v*))	*Integrated point* (*log* (*ng day cm*$^{-2}$))	*Integrated disc* (*log* (% *w/v day*))
JF8133 formulation				
Transport coefficient $\times 10^{-10}$ (cm^2 s^{-1})	2·59	3·69	3·89	6·60
Log LD_{50}	2·33	−1·92	7·85	−1·90
Standard deviation	1·68	1·15	1·49	0·99
VK1 formulation				
Transport coefficient $\times 10^{-10}$ (cm^2 s^{-1})	5·45	5·25	10·85	10·53
Log LD_{50}	3·50	−1·38	8·98	−1·43
Standard deviation	0·59	0·60	0·55	0·56

centre, the concentration merely rises with time. Both point and disc source models can be adapted to allow for the accumulated effect of toxicant on the organisms over time. This can be achieved by numerical integration of the appropriate form of the diffusion model over time and using this integrated exposure (dose × time) as the metameter in the log tolerance distribution.

Figure 4 shows plots of the integrated exposure forms of the point source model for a 114 μm diameter droplet containing 100 g litre^{-1} permethrin in JF8133 formulation. The integrated forms of the model fit the experimental data more closely near the limits of the mortality scale (i.e. in the tails of the distribution of responses). This is important since insecticide treatments are usually designed to achieve 95% or more pest mortality. Over a broad range either side of the median response, however, there is little to choose between the models. Similar results were obtained for VK1 at different drop sizes and concentrations.

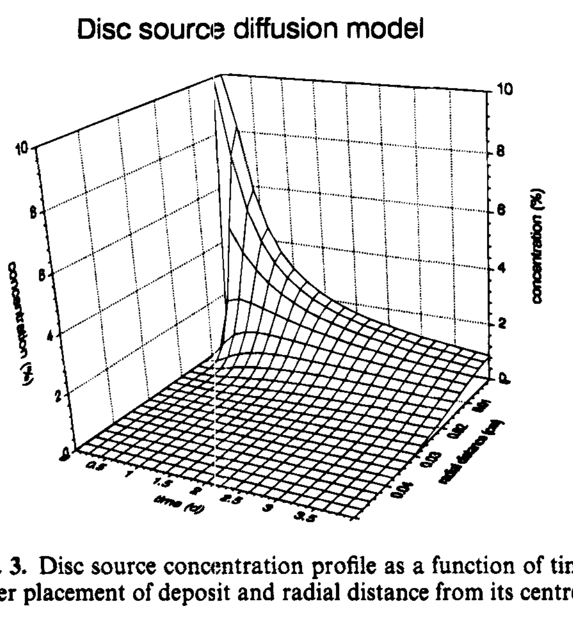

Fig. 3. Disc source concentration profile as a function of time after placement of deposit and radial distance from its centre.

3.3 Choice of an appropriate model for further studies

The parameters of the various models estimated for the two permethrin formulations, JF8133 and VK1, using non-linear regression of proportion mortality on radial distance are presented in Table 1. The *a priori* notion that the more complex forms of the diffusion model would provide for better fits of the data was not borne out by these results. This is also established in Fig. 5(a)

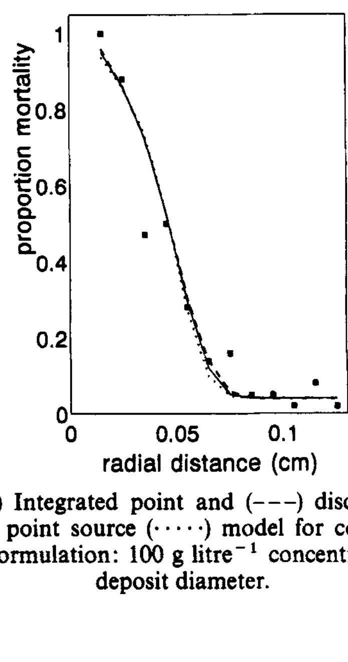

Fig. 4. (——) Integrated point and (– – –) disc models (with the ordinary point source (·····) model for comparison) for the JF8133 formulation: 100 g litre^{-1} concentration, 114 μm deposit diameter.

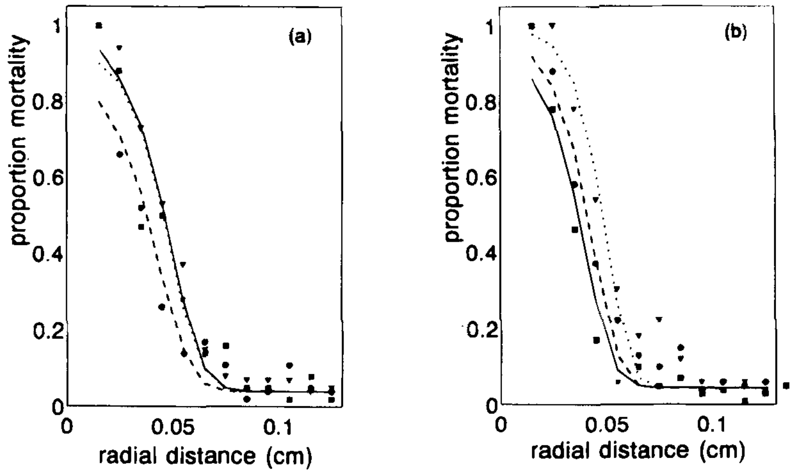

Fig. 5. Point source model concentration profiles fitted to experimental data: (a) JF8133 formulation: 100 g litre^{-1} concentration for (--●--) 59, (··▼··) 108 and (—■—) 114 μm deposit diameter; (b) VK1 formulation: (—■—) 50, (--●--) 100 and (··▼··) 200 g litre^{-1} concentrations for 107, 110 and 113 μm deposit diameters respectively.

which presents data for a fixed concentration of the JF8133 formulation of permethrin to show that the point source model can predict the whitefly mortality observed for deposits of different size; Fig. 5(b) presents a similar plot for the VK1 formulation to show that the point source model is able to predict the mortality observed for changes in the concentration of permethrin for deposits of approximately constant size. Thus, for a variety of conditions, the point source model gives an adequate description of the poisoning process.

Since the mathematics of this model lead to an analytical solution which is easier to compute, it has been used as the basis for further studies. It should be noted, however, that the disc source model provides a more realistic representation of the transfer process and that its parameters have units (Table 1) which are more straightforward to interpret.

3.4 Proportion of leaf area cover maintained at a given level of control

From eqn (1), and assuming negligible overlap of the regions of influence around the insecticide deposits, it can be seen that the total leaf area protected to at least 50% control with a fixed volume of spray is given by $\pi r_{50}^2 N R_f$. Thus, the proportion P of the total spray area A with this level of control can be expressed as

$$P = \frac{\pi r_{50}^2 N R_f}{A} = \frac{3LDtR_f}{Aa^3}\left[\ln\left(\frac{C_0 a^3}{3Dt10^6}\right) - \mu\right]10^{15} \quad (5)$$

which is eqn (12) of Sharkey *et al.*[9] Rewriting eqn. (5) to make C_0, the concentration of AI in the deposit at time $t = 0$, the subject of the expression, we have

$$C_0 = \frac{3Dt}{a^3}\exp\left\{\frac{PAa^3}{3LDtR_f 10^{15}} + \mu\right\}10^6 \quad (6)$$

C_0 can now be plotted as a function of the inflight droplet radius, a. Figure 6 presents this relationship obtained for $P = 1$ (100% of the spray area protected to at least 50% control), $L = 5$ (5 litres of spray) and $A = 1$ hectare, $t = 4$ days, assuming a leaf area index of one and 100% retention of the spray droplets by the leaf surface. This latter condition, although unrealistic, serves to demonstrate the properties of the model. Under field conditions, a retained fraction less than 0.6 is commonly observed; the result of reducing this quantity is predicted by eqn (6). If $R_f = 0.5$, for example, the first term in the exponent will double to result in a substantially higher predicted value for C_0 and a reduced optimal drop size ($\times 0{\cdot}79$: see equation below). The values of D and μ used were those obtained from the non-linear regression (Table 1) for the JF8133 formulation of permethrin applied to tobacco leaves for the control of whitefly larvae (point source model). The C_0

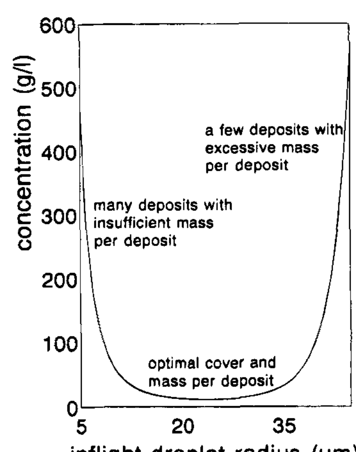

Fig. 6. Initial concentration of C_0 of AI required to obtain a given level of control over a known proportion of the crop surface (see text for details) as a function of deposit size, assuming no overlap.

curve falls rapidly as the droplet radius is reduced (the result of an increased cumulative deposit perimeter and therefore a larger front for pesticide movement) to describe a very flat-bottomed profile around a minimum value of C_0, before rising again as the droplet radius is further reduced (the consequence of insufficient AI in each deposit to maintain the concentration in the 'zone of diffusion' surrounding the deposit above that required for control of the pest). This concentration profile suggests that if a fixed volume of spray is deposited over a finite leaf area, an optimal in flight droplet size is required to reduce the amount of AI to a minimum. The point source model assumes that once a droplet has impacted on a plant surface its radius is unimportant other than to determine the mass of AI contained therein. The optimal droplet radius for this minimum occurs at $a = [(3LDtR_f/A)10^{15}\}]^{1/3}$ which, for this example, is approximately 24 μm. However, biocidal efficacy is predicted to vary little between 16 and 32 μm deposit radius. It should be noted that, because the point source model cannot utilise information about droplet spread, formulation effects mediated through droplet spreading cannot be considered. However, for such a study the disc source model would be appropriate. Moreover, optimal droplets may require in-flight diameters associated with significant levels of drift. In such cases, a compromise may be necessary, e.g. by choosing the smallest drop size which gives an acceptable level of drift.

3.5 Determination of the number of droplets per unit area causing median mortality

Adams *et al.*[7] suggest that the number of droplets per unit area (LN_{50}) which will result in 50% response provides a useful measure for assessing the efficacy of a treatment. Their results, based on studies of isolated deposits of permethrin applied at ULV for the control of whitefly larvae on tobacco, are reproduced in Fig. 7. This figure shows the change in LN_{50} as a function of inflight droplet radius a (15–54 μm) for a 100 g litre^{-1} solution of the JF8133 formulation of permethrin. Because of the cubic relationship between droplet diameter and its volume and hence the quantity of AI there is an approximate 12-fold reduction in the amount of material per unit area, i.e. the LQ_{50} (from 1·65 to 0·14 μg cm^{-2}) compared with a 10-fold reduction in that predicted for Adam's data by eqn (6), assuming 100% spray retention.

Munthali and Scopes 'assumed that a 50% kill means that 50% of the leaf is toxic to the test organism'.[10] This situation can be modelled by considering a leaf surface covered by a hexagonal array of deposits[7] such that in the area around them there is, on average, 50% control. For this arrangement the problem of predicting the LN_{50} then reduces to finding the interdeposit distance

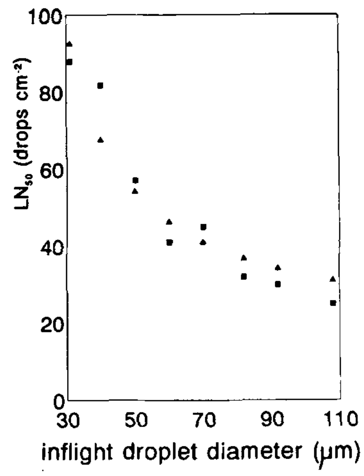

Fig. 7. Changes in (■) observed and (▲) predicted LN_{50} values of whitefly larvae resulting from changes in the inflight deposit diameter of 100 g litre^{-1} JF8133 formulation of permethrin ($D = 7{\cdot}5 \times 10^{-10}$ cm^2 s^{-1}, $\mu = 1{\cdot}9$ log(ng cm^{-2}), $\sigma = 1{\cdot}7$ log(ng cm^{-2}), control mortality = 7%).

$2d$ (Fig. 8) which results in 50% control over the entire sprayed surface. However, in order to obtain an unbiased estimate of the LN_{50} the influence on biocidal activity of overlapping regions of pesticide arising from neighbouring deposits must be considered.

Figure 8 shows diagramatically the arrangement of three nearest-neighbour deposits. Because of symmetry, the triangular area AOD (Fig. 8) constructed in the equilateral triangle ABC (with sides of length $2d$) characterised by the nearest-neighbour deposits centred at A, B and C forms the basic unit of calculation for this idealised hexagonal arrangement. On the assumption that the only significant contributions to be made to the concentration of AI in this smaller triangle will be from the deposits centred at A, B and C, the mass of AI per unit area anywhere in this triangle (say w) may be found by summing the point source model ($C^*(r, t)$) evaluated

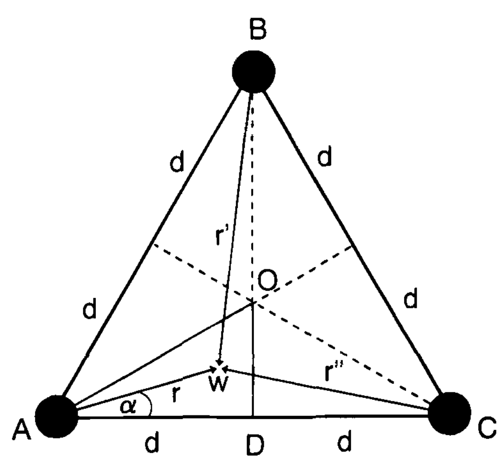

Fig. 8. Diagrammatic representation of three nearest-neighbour deposits, showing the radial distances to a general point w in the triangular region AOD.

at the radial distances r, r' and r'' (see Fig. 8), where

$$r'^2 = r^2 + 4d^2 - 4rd\cos(\alpha)$$
$$r''^2 = r^2 + 4d^2 - 4rd\cos(\pi/3 - \alpha)$$

and where α is the angle that the radius vector r makes with the line AD.

The interdeposit distance is calculated as follows. Take the line AO (hypotenuse of triangle AOD) which is of length $2d/\sqrt{3}$ and divide it up into k equal intervals (k integer) so that the $k + 1$ radii $r_0, r_1, r_2, \ldots, r_k$ can be defined as

$$r_0 = 0,\quad r_1 = \frac{2d}{k\sqrt{3}},\quad r_2 = 2\frac{2d}{k\sqrt{3}},\quad r_k = k\frac{2d}{k\sqrt{3}} = \frac{2d}{\sqrt{3}}.$$

Similarly, take the angle OAD $= \pi/6$ and divide into n equal angles (n integer) so that the $n + 1$ angles $\alpha_0, \alpha_1, \alpha_2, \ldots, \alpha_n$ can be defined as

$$\alpha_0 = 0,\quad \alpha_1 = \frac{\pi}{6n},\quad \alpha_2 = 2\frac{\pi}{6n},\quad \alpha_n = n\frac{\pi}{6n} = \frac{\pi}{6}.$$

Assuming that the organisms are distributed randomly over the leaf surface at a density of λ per unit area, then the number of organisms in the partial annulus r_{j-1} to r_j, α_{i-1} to α_i is given by

$$\lambda\pi(r_j^2 - r_{j-1}^2)\frac{(\alpha_i - \alpha_{i-1})}{2\pi}$$

If the proportion of organisms responding at a radial distance r_j from deposit A and angle α_i from the line AD is denoted by $p(r_j, \alpha_i)$, then for sufficiently large k and n, the number of organisms in the partial annulus r_{j-1} to r_j, α_{i-1} to α_i responding may be approximately stated,

$$\lambda\pi(r_j^2 - r_{j-1}^2)\frac{(\alpha_i - \alpha_{i-1})}{2\pi}p(r_j, \alpha_i)$$

so that the total number responding in the triangular area AOD is given by

$$\sum_{j=1}^{k}\sum_{i=1}^{n}\lambda(r_j^2 - r_{j-1}^2)\frac{(\alpha_i - \alpha_{i-1})}{2}p(r_j, \alpha_i)$$

From the interpretation of biocidal area suggested by Munthali and Scopes,[10] it follows that dividing the total number of organisms responding by the total number of organisms in the area AOD, i.e. $\lambda d^2/2\sqrt{3}$ and setting this to 0·5 (50% response; $P = 0{\cdot}5$), gives eqn (7) from which d may be determined.

$$\sum_{j=1}^{k}\sum_{i=1}^{n}(r_j^2 - r_{j-1}^2)\frac{(\alpha_i - \alpha_{i-1})}{d^2/\sqrt{3}}p(r_j, \alpha_i) = 0{\cdot}5. \tag{7}$$

Taking the limit $k \to \infty$, $n \to \infty$, d is then the solution of the equation

$$\int_0^{(2d/\sqrt{3})}\int_0^{\arcsin(d/r)}\frac{2\sqrt{3}}{d^2}rp(r, \alpha)\,dr\,d\alpha = 0{\cdot}5. \tag{8}$$

LN_{50} values can now be approximated as $1/\pi[(d + 2d/\sqrt{3})/2]^2$ where $(d + 2d/\sqrt{3})/2$ is the average of the two distances AD and AO, respectively in Fig. 8.

Figure 7 presents the predicted LN_{50} values obtained assuming overlapping biocidal areas and those observed from the work of Adam's *et al.*[7] plotted against deposit diameter. The predictions are in reasonable agreement with the experimental observations, providing a useful validation of the derived model. The biases in the predicted LN_{50} values at high droplet diameter, on average approximately 5 cm^{-2}, are within the errors of field application. This result therefore suggests that it should be possible to use the extended model to predict the efficacy of controlled droplet applications of known deposit size, concentration and deposit density.

Figure 9 presents profiles obtained for four different volumes of application using the parameters estimates obtained for the data of Adams *et al.*[7] (Fig. 7). Thus, the model modified to take account of overlapping biocidal areas gives broadly similar concentration/drop size pro-

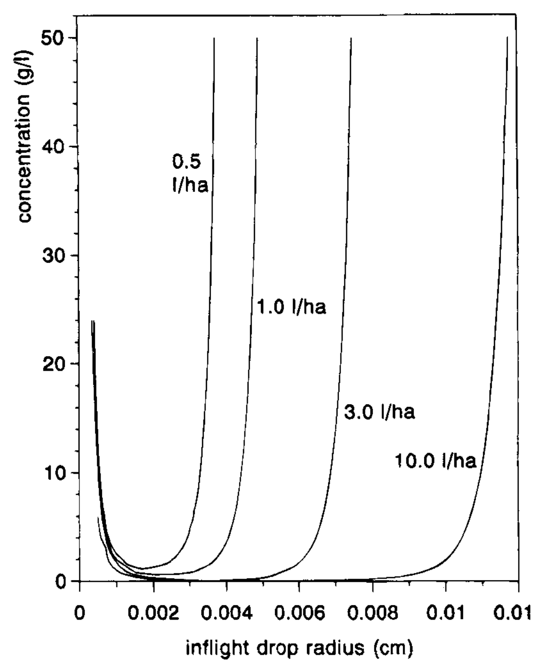

Fig. 9. Initial concentration C_0 of AI required for the four volumes of application shown to obtain a given level of control over a known proportion of the crop surface as a function of deposit size, assuming overlapping biocidal areas.

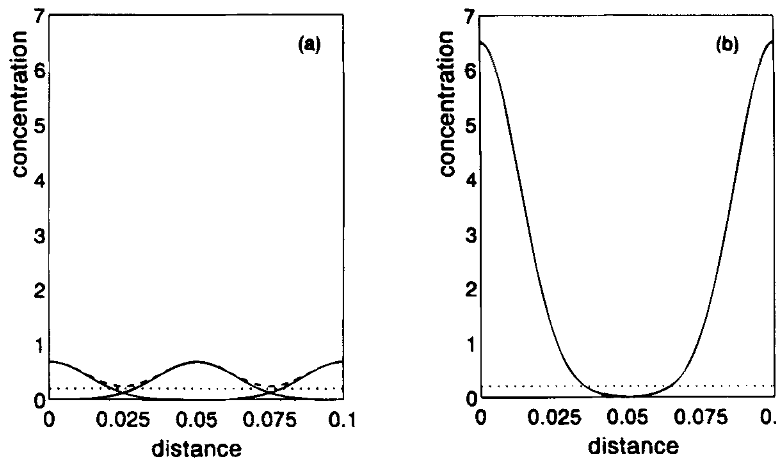

Fig. 10. Simulated four-day concentration (arbitrary units) profiles for (——) nearest-neighbour deposits, (- - -) their combined (summed) effect, together with (· · · · ·) the threshold level for (a) three (nine deposits per unit area) low-concentration (one concentration unit) deposits, and (b) two (four deposits per unit area) high-concentration (10 concentration units) deposits.

files to that reported for negligible overlap in Fig. 6. Furthermore, it can be seen that the range of drop sizes which produce a fixed level of control (50% control over the entire leaf surface) at a minimum spray concentration, increases with increasing volume of application. Sprayers producing a wide range of drop sizes, e.g. those fitted with hydraulic nozzles, are predicted to require larger volumes of application than sprayers, e.g. spinning disc sprayers, which produce a narrow band of drop sizes. This establishes the unsuitability of conventional spraying equipment for ULV application. Figure 9 also highlights the potential of mathematical modelling of pest/pesticide interactions for designing appropriate control strategies since optimal treatment combinations (concentration of AI, volume application rate and drop size) can readily be identified. As already noted (Section 3.4), a compromise between what is optimal and what can actually be achieved commercially under field conditions is sometimes necessary.

3.6 Discriminating biocidal efficacies

A number of interesting observations relating to the leaf area covered by pesticide deposits and the timing of applications have emerged from the modelling studies. It may be possible, for example, to identify deposits with discriminating biocidal efficacies. The experimental data relating to leaf cover establish that a very small proportion of the leaf surface is covered by spray deposits. However, because of the zones of influence around the deposits, a high level of control is achieved over a substantial area of the leaf surface. A comparison of these areas shows that they can be approximately 20 to 100 times as large as the spread deposit depending on concentration and drop size, with the upper end of the range being achieved for the smaller drop sizes. As it is felt that the AI is moving out from the deposit within the leaf cuticle, and is therefore unavailable at the plant surface, this result is of considerable interest, in that beneficial insects walking over these regions may be less likely to contact and pick up a toxic dose. Furthermore, pesticide can be dissipated from the centre of even concentrated deposits quite rapidly, as a result of its random movement away from the deposit through the plant cuticle (Fig. 3), again making it less available to surface dwellers. Thus, treatments designed for high biocidal efficacy (i.e. large areas of control per unit mass of pesticide) against sedentary pests such as whitefly larvae, which are in intimate contact with the plant cuticle, may be relatively innocuous to many non-target organisms and therefore able to discriminate between pests and beneficials. This hypothesis is speculative, however, and requires experimental confirmation. For some insecticides, for example, the vapour activity from deposits could have some impact on populations of beneficials occupying niches within range of treated plant surfaces. In addition, vapour loss and foliar penetration could both modify the availability of AI to non-target insects.

The above observations assume that the impacted deposit maintains a constant radius, a. However, the physicochemical properties of the deposit, which will depend on the nature of the AI and the particular formulation used,[11] and those of the plant surface on which deposit is resting will also influence the zone of influence. For example, permethrin used in this study is a low-melting-point liquid which on deposit ageing can slowly crystallise to form a solid. Other AIs have much higher melting points and may be applied as particles, e.g. as SC or WP formulations. Such factors may modify the initial movement of AI from the deposit. Because the distances between particles of AI within a deposit are small compared with those between deposits, however, these effects are unlikely to have undue influence on the outcome measured over days or weeks after spray application.

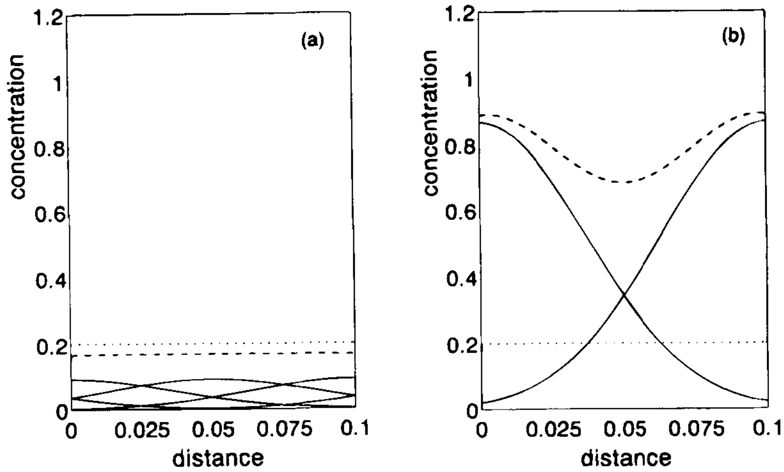

Fig. 11. Simulated 30-day concentration (arbitrary units) profiles for ——) nearest-neighbour deposits, (– – –) their combined effect, together with (· · · · ·) the threshold level for (a) three (nine deposits per unit area) low-concentration (one concentration unit) deposits, and (b) two (four deposits per unit area) high-concentration (10 concentration units) deposits.

3.7 Increasing the duration of control using minimal pesticide input

It is sometimes necessary to recommend treatments for situations where it is difficult or impossible to undertake appropriate experiments. Analytical models of insecticide action may provide a rationale to suggest how to apply insecticides most effectively under such conditions. This is particularly appropriate when, as in the present study, the models have been tested and validated. Such models may also be useful when comparing potential strategies prior to experimentation.

Consider the problem of achieving the maximum duration of control of a sedentary pest using a minimum applied dose. To achieve the desired control of a sedentary pest, it is necessary to maintain the deposit above some threshold dose per unit area for the period required to protect the crop. Any deposit will have a finite life because the mass of AI applied per unit area of plant surface will eventually fall below the threshold for control.

The deposit characteristics for short-term control are different from those required at longer times after spraying. This point is illustrated graphically in Figs 10–12 where the difference in terms of cover that can be achieved at two time points (four and 30 days) with high density (nine deposits per unit area) low-concentration (one concentration unit) sprays and low-density (four deposits per unit area), high-concentration (10 concentration units) sprays is shown. The concentration profiles obtained for each time can be summed to calculate the insecticide cover in the regions of deposit overlap.

Let us consider some arbitrary threshold cover at say 0·2 (arbitrary units) as the level required for 'protection' over all the leaf surface. After four days, the combination of low concentration and high deposit density attains the critical threshold over the entire leaf surface (Fig. 10a), whereas the high-concentration/low-deposit-density treatment remains below this level over much of the target area (Fig. 10b). By 30 days the situation has been reversed (Fig. 11). The low-concentration deposits are now predicted to fall below the threshold level (Fig. 11a) because diffusion of material depletes insecticide at the surface (the model assumes an infinite surface area) whereas the high-concentration deposits are considerably in excess of the critical threshold over the entire spray area (Fig. 11b). However, although effective, the latter treatment uses unnecessarily large amounts of insecticide. Adequate control during the 30-day period can be obtained using less material simply by increasing the number of low-concentration deposits from nine to 25 per unit area as illustrated in Fig. 12 (vertical scale expanded) to result in 25/40ths of the applied dose at the high-concentration treatment. The study also suggests that increased duration of control at minimal dose

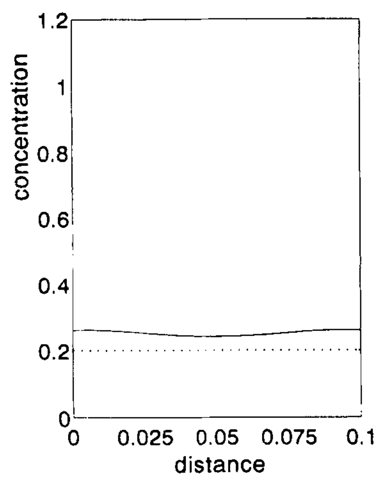

Fig. 12. Simulated 30-day concentration (arbitrary units) profiles for (——) five (25 deposits per unit area) nearest-neighbour low-concentration (one concentration unit) deposits, (– – –) their combined effect together with (· · · · ·) the threshold level.

may result from the use of composite sprays which combine appropriate numbers and sizes of high and low concentration deposits.

4 CONCLUSIONS

Earlier models defining optimal deposits for the control of sedentary pests have been extended and further validated. The studies suggest that the point source and disc source models provide adequate descriptions of the factors which determine biological efficacy of CDA applications for the control of sedentary arthropod pests. Estimates of the transfer coefficients for lateral pesticide movement through plant cuticles and the distribution of tolerances of sedentary target species in their natural condition have now been obtained for the disc source model. Integrated forms of both the point and disc source models give better descriptions of the control in the extremes of the tolerance distribution (high and low mortalities) where attention must be focused when designing strategies to control pests but protect non-target organisms. Identification of optimum deposits suggests how pesticide inputs may be reduced while maintaining control of the pest in a manner which ensures minimal hazard to the biological agents used in IPM. For a fixed volume of application, an optimum deposit size can be predicted which minimises the amount of AI required for at least 50% response over the leaf surface. Although ignoring the influence of formulation composition, spread after impaction and subsequent bioavailability, this prediction is consistent with the experimental observations of Adams *et al.*[7] Furthermore, the number of deposits required for 50% control has been predicted to decrease with increasing drop size in a manner consistent with observation.[7] Modelling studies also suggest that chemical inputs may be reduced by the application of composite sprays of mixed droplet characteristics, targeted for immediate and longer-term control of arthropod pests. The analytical models described in this paper may be useful in the design of crop protection treatments for use against other sedentary targets, e.g. for the control of weeds and diseases by contact herbicides and fungicides. However, practical limitations restrict the types of spray application which can currently be adopted for a particular crop protection problem. Improved delivery systems may therefore be necessary before the full benefits of a modelling approach can be realised.

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